Finite liquid drop size effects on the $d = 2$ Ising square lattice

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Finite size effects are essential in the study of nuclei and other mesoscopic systems. In cluster physics, finite size effects arise when relating properties of the infinite system to clusters. In nuclear physics finite size effects dominates and the challenge is generalize properties of the nucleus to a description of bulk nuclear matter.

Physical cluster theories of non-ideal vapors, with clusters, state that the concentrations of vapor clusters of A constituents $n_A(T)$ depend on the cluster formation free energy $\Delta G_A(T) = \Delta E_A(T) - T\Delta S_A(T)$. At coexistence, $\Delta E = c_0 A^\sigma$ and $\Delta S_A(T) = \frac{c_0}{T_c} A^\sigma - \tau \ln A$ [1]. Thus

$$n_A(T) = \exp\left[-\frac{\Delta G_A(T)}{T}\right] = q_0 A^{-\tau} \exp\left(-\frac{c_0 A^\sigma \varepsilon}{T}\right) \quad (1)$$

q_0 is a normalization, τ is the topological exponent, c_0 is the surface energy coefficient, σ is the surface to volume exponent, and $\varepsilon = (T_c - T)/T_c$. The term in $\Delta S_A(T)$, proportional to A^σ, permits the vanishing of the cluster free energy at a $T = T_c$. We generalize eq. (1) to the case of a vapor in equilibrium with a finite liquid drop. We extract each vapor cluster from the liquid, determining entropy and energy changes of the drop and cluster, and then put it back into the liquid, as if, according to physical cluster theories, no other clusters existed. Then $\Delta E_A(T)$ and $\Delta S_A(T)$ can be written for a drop of size $A_{\rm d}$ in equilibrium with its vapor as $\Delta E_A(T) = c_0\left[A^\sigma + (A_{\rm d} - A)^\sigma - A_{\rm d}^\sigma\right]$ and $\Delta S_A(T) = \frac{c_0}{T_c}\left[A^\sigma + (A_{\rm d} - A)^\sigma - A_{\rm d}^\sigma\right] - \tau \ln\left[A(A_{\rm d} - A)/A_{\rm d}\right]$ giving

$$\begin{aligned} n_A(T) \;&=\; q_0\left[A\,(A_{\rm d} - A)/A_{\rm d}\right]^{-\tau} \\ &\exp\left\{-c_0\varepsilon\left[A^\sigma + (A_{\rm d} - A)^\sigma - A_{\rm d}^\sigma\right]/T\right\}. \quad (2) \end{aligned}$$

The free energy cost of complement $(A_{\rm d} - A)$ formation is determined just as the free energy cost of cluster (A) formation is determined. Equation (2) reduces to eq. (1) *when* $A_{\rm d}$ *tends to infinity* and contains the same parameters. We can rewrite eq. (2) as $n_A(T) = n_A^\infty(T)\exp\left(A\Delta\mu_{\rm fs}/T\right)$ with $n_A^\infty(T)$ given by eq. (1). The finite size of the drop acts as an *effective* chemical potential, $\Delta\mu_{\rm fs} = -\left\{c_0\varepsilon\left[(A_{\rm d} - A)^\sigma - A_{\rm d}^\sigma\right] - T\tau\ln\left[(A_{\rm d} - A)/A_{\rm d}\right]\right\}/A$.

To demonstrate this method, we apply it to the canonical lattice gas (Ising) model on the square lattice with a fixed number of up spins $A_{\rm d}^0$ (fixed magnetization $M_{\rm fixed}$ Ising model) [2]. We examine the scaled cluster concentrations: $n_A(T)/q_0 A^{-\tau}$ vs. $c_0 A^\sigma \varepsilon/T$. For $M_{\rm free}$ calculations this scaling collapses cluster concentrations [3]. Finite liquid drop size effects appear in the $M_{\rm fixed}$ cluster concentrations which scale better with eq. (2) than eq. (1). To compare the $M_{\rm free}$ cluster scaling and with the $M_{\rm fixed}$ cluster scaling, we fit the $M_{\rm free}$ clusters to eq. (1) with free parameters T_c, c_0, σ and τ; $q_0 = \zeta(\tau - 1)/2$. See Table I and Fig. 1. Next we calculate χ^2_ν for the $M_{\rm fixed}$ clusters using eq. (1) and eq. (2) with parameters fixed to the Table I. The $M_{\rm fixed}$ χ^2_ν values for eq. (2) are an order of magnitude smaller than the results for eq. (1) and the data collapse is better.

TABLE I: Fit results

	$M_{\rm free}$		$M_{\rm fixed}$			
-	Onsager	this work				
χ^2_ν	-	4.7				
T_c	2.26915	2.283 ± 0.004				
c_0	≥ 8	8.6 ± 0.2	$A_{\rm d}^0$ $(d=2)$	640	320	160
σ	8/15	0.56 ± 0.01	χ^2_ν eq. (1)	10.3	10.6	18.2
τ	31/15	2.071 ± 0.002	χ^2_ν eq. (2)	1.7	1.9	4.8

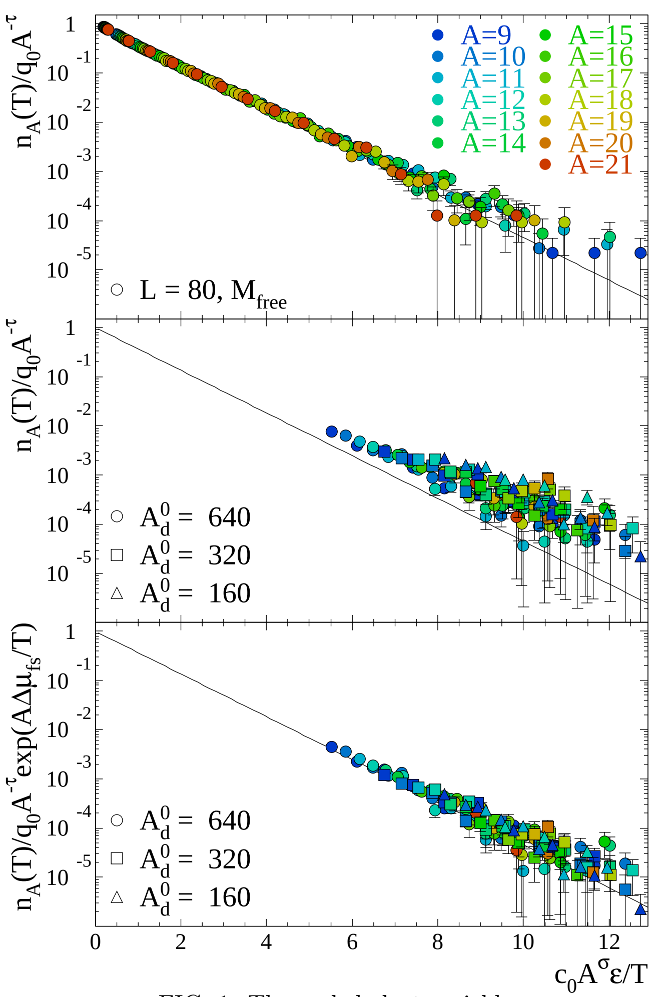

FIG. 1: The scaled cluster yields.

[1] M. E. Fisher, Rep. Prog. Phys. **30**, 615 (1967).
[2] L. G. Moretto *et al.*, Phys. Rev. Lett. **94**, 202701 (2005).
[3] C. M. Mader *et al*, Phys, Rev, C **68**, 064601 (2003).